METHODOLOGY DEVELOPMENT FOR MEASUREMENT OF AGENT FATE IN AN ENVIRONMENTAL WIND TUNNEL

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Abstract. The environmental fate of chemical warfare agents on targeted surfaces is important in modeling vapor and contact hazard for decisions influencing safety of personnel in contaminated areas. Several laboratory wind tunnels are under development and include microbalance, vapor sampled, and contact angle wind tunnels. A wide spectrum of methodology development is required to control and measure physical parameters and analyte mass distribution. The methodology developed to date will be described and examples provided.

INTRODUCTION

Hazard prediction models (1) require a database of chemical agent desorption rates as a function of agent type, surface composition, droplet size, wind speed, temperature, relative humidity, and other variables. A spectrum of methods for the analysis of the contaminants throughout a mass balance process is also required. Vapor sampling and analysis methods are required to monitor the vapor flux from the droplet; this includes a requirement for interleaved calibration. Solvent extraction methods are required for quantification of the residual agent in several porous substrates; substrates include concrete, asphalt, aggregate from concrete and asphalt, soil, and nonporous metal or glass controls. Methods for monitoring the environmental variables that influence transport rates must be developed for use in a toxic chemical agent wind tunnel. These include measurement of the wind speed and flow profile at ground level, near the droplet, and at the wind tunnel centerline. In addition, the overall flow rate within the wind tunnel must be measured to compute the vapor concentration. Flow rates and pressure differentials must be balanced during switching between the sampled and non-sampled periods. Temperature and relative humidity must be measured at the source and near the chemical agent droplet. The vapor sampling procedure must ensure that the sampled agent is homogeneously mixed at the sampling point. Optical imaging of the droplet or wetted area must be synchronized with the other data acquisition measurements. The overall data acquisition strategy must record the timing of each measurement to align agent concentration with environmental variables. The development of these methodologies is underway and results to date are presented.

The goal is to provide data sets to allow development of improved models for hazard predictions, supporting decisions on personnel safety. An environmental microbalance wind tunnel was previously show to be useful for chemical agent measurements (2). The scale of the program includes 3 levels: laboratory, chamber, and field. In order to cover different regimes of the experimental design, several different laboratory wind tunnel types are being developed, each with different cross-sectional areas: microbalance, vapor-sampled, and contact angle wind tunnels. The material surfaces and droplet geometries include the study of nonporous, sessile droplet geometry *versus* porous, sorbed droplet shape and spread factor geometries.

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The development of unique methodologies is required for a toxic chemical wind tunnel:

- The safe dosing of chemical agents on environmental surfaces within a wind tunnel.
- The accurate control of droplet size.
- Control and measurement of air temperature from the environmental control source to the droplet.
- Control and measurement of air relative humidity from the environmental control source to the droplet: avoiding condensation on cool surfaces
- Control and measurement of the wind speed near the chemical agent droplet
- The vapor analysis of chemical agents with a wide concentration range.
- The integration and coordination of time dependent measurements for physical, chemical and imaging data

The experimental matrix can be divided into several categories of variables. The chemicals include HD, GD, thickened GD, VX, and thickened VX. The material surfaces are concrete-mortar, concrete-aggregate, asphalt-bitumen, asphalt-aggregate, sand, soil, and a reference surface of glass or aluminum. The physical parameters include drop size, temperature, humidity (relative and absolute), and wind speed at the drop/material interface.

RESULTS

Design and Control of Environmental Parameters. A photograph of an interim design (3) of a toxic chemical wind tunnel shows (Figure 1) a 5 cm-square wind tunnel of stainless steel material. The versatile design can be configured in two analytical regimes, total analyte collection or sampled collection, and can be dismantled in sections for decontamination.

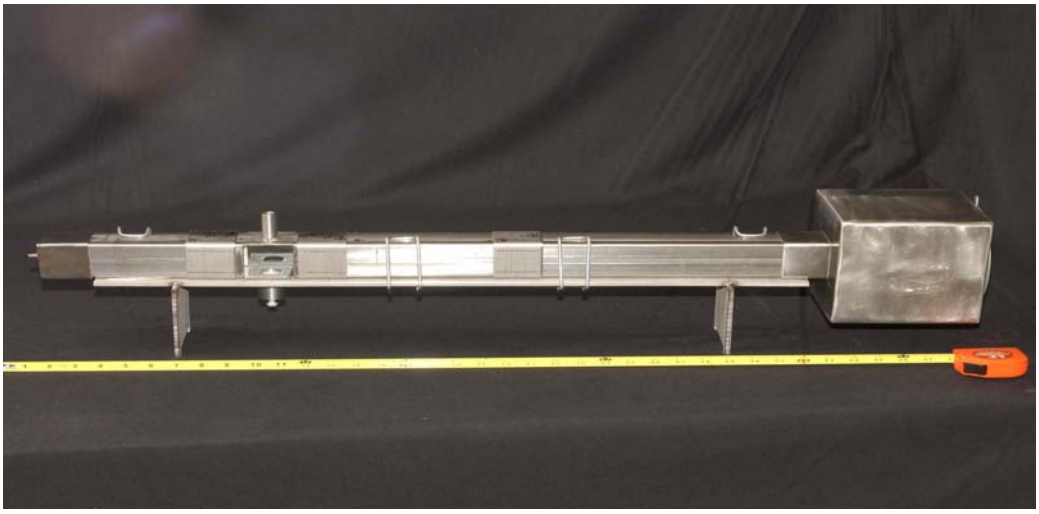
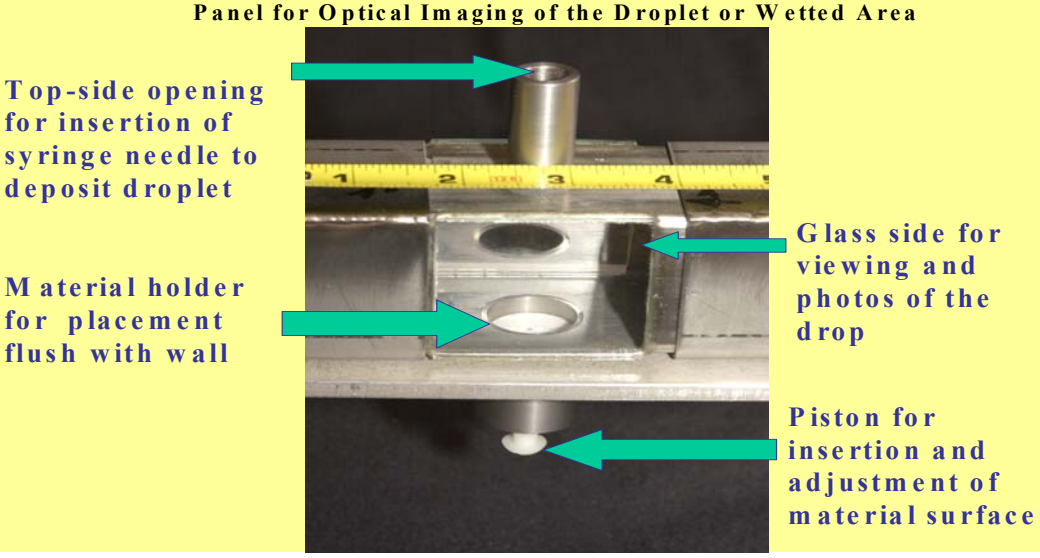


FIGURE 1. Photograph of a Toxic Chemical Lab Wind Tunnel: A 5-cm Square by 1 Meter Version Configured in a Low Wind Speed, Total Analyte Collection Mode.

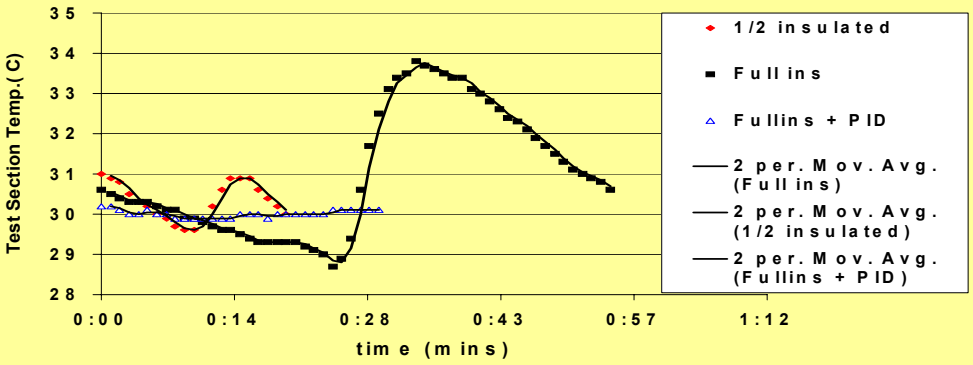
A close-up photograph of the wind tunnel Test Section shows (Figure 2) the topside opening for deposition of the droplet by syringe or pipette, before sealing with a cover. The adjustable cylinder allows placement of the material surface flush with the wind tunnel floor. The parallel glass sides allow illumination and optical imaging of the droplet profile or wetted area.

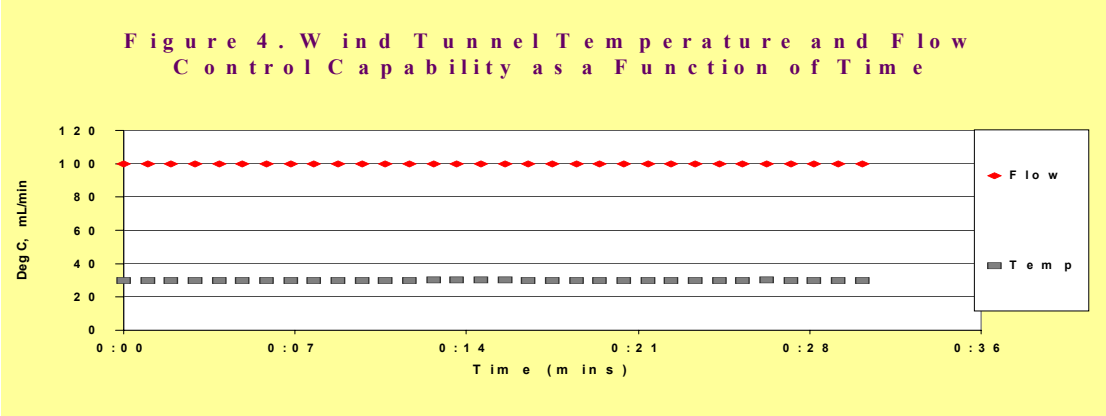
Figure 2. Photograph of the Test Section of the Wind Tunnel Showing the Top-side Droplet Deposition Opening, the Material Surface Holder, and Glass Side Panel for Optical Imaging of the Droplet or Wetted Area



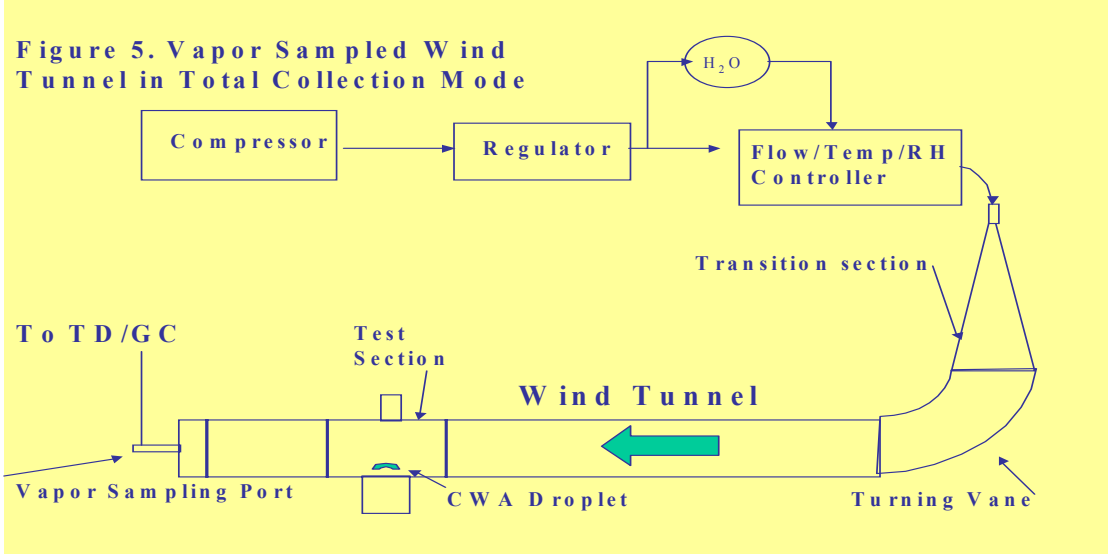
A comparison of several thermal control strategies is provided (Figure 3); as insulation level is increased and temperature control is improved with a PID algorithm, the deviations from the set point decrease. The most recent temperature and flow control performance is shown in Figure 4.

Figure 3. Comparison of Wind Tunnel Temperature Control Fluctuations for Competing Temperature Control Algorithms and Insulation Geometries





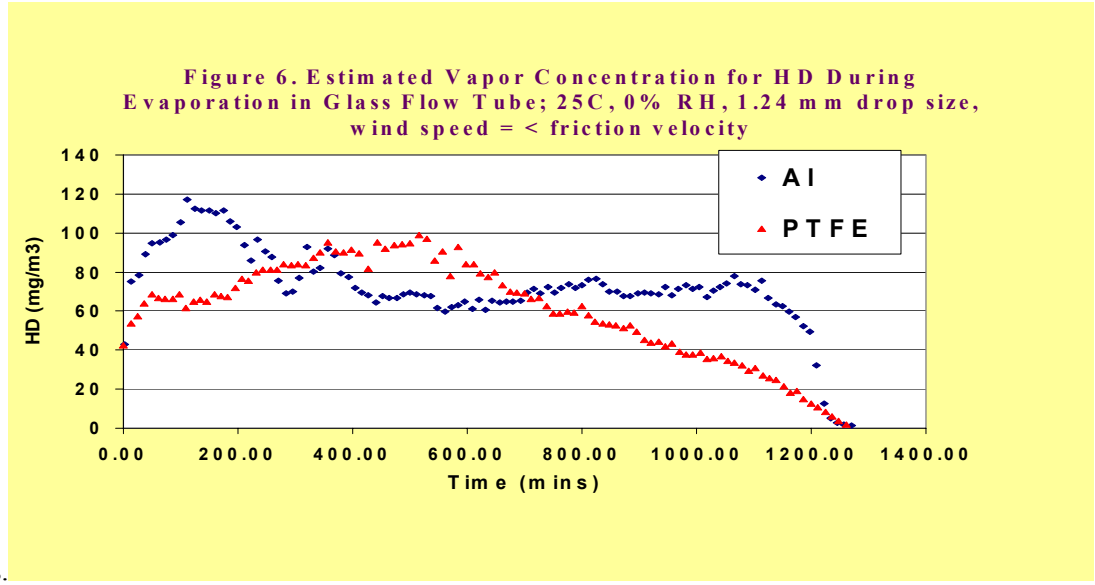
Vapor Analysis Methodology Results. A diagram in Figure 5 shows the vapor sampled wind tunnel in total collection mode. The wind speed is generated by a pump driven 'Pull' from the thermal desorber system augmented by a passive source of conditioned air from the environmental controller via a custom molded transition section and turning vane. A flow straightening section is followed by turbulence trips and the test section. The entire flow stream exits through the vapor sampling port to the thermal sorption/desorption tube (TD) and gas chromatograph (GC).



Diagnostic experiments were performed to evaluate selected performance criteria of the vapor analysis system to guide analytical improvements. A tubular glass wind tunnel was employed to measure HD evaporation under identical temperature (25 deg C), relative humidity (~0%) and wind speed (< friction velocity) from two contrasting substrates, polar aluminum (Al) and nonpolar polytetrafluoroethylene (PTFE). The Unity (Markes Ltd) thermal desorber (TD) and GC system were employed.

Observations revealed that HD spreads to a film-like geometry on aluminum while HD retained a sessile drop geometry on PTFE, as expected. The HD/Al plot of concentration versus time shows a rather constant evaporation rate demonstrated by the concentration values plotted parallel to the time axis in Figure 6. The derivative curve in Figure 6 shows the HD/PTFE plot with a curvature,

often representing a change of drop surface area with time. Figure 7 shows a near zero-order linear plot in the integrated form of the plot in Figure 6. Overall, the wind tunnel combined with the analytical system demonstrated the ability to discriminate between sessile droplet evaporation from differing surface area geometries.



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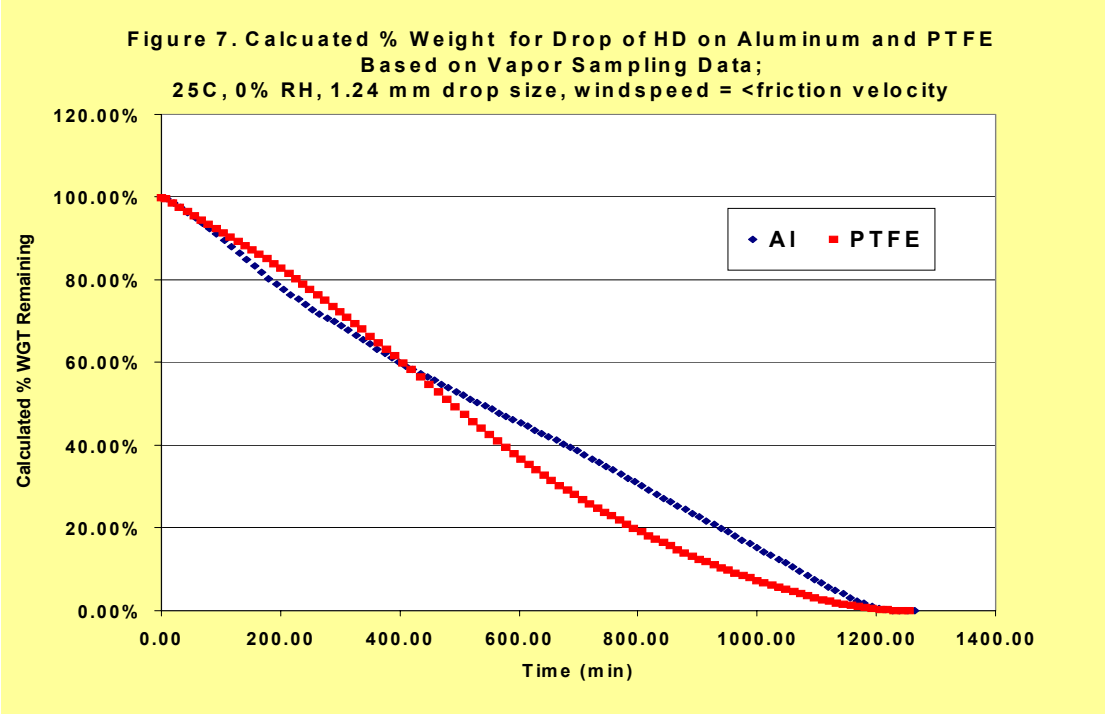


A parallel example is provided in the plots of concentration versus time for HD evaporation from aluminum shown in Figures 8 and 9, except a different combination of wind tunnel and vapor

analysis system were employed. The 5-cm stainless steel wind tunnel (see Figure 1) was coupled to a thermal desorption system and GC/MS (Inficon Hapsite Model). The temperature was 30 deg C; the relative humidity was ca 0%, and the drop size 1.27 mg or 1 uL. The plot in derivative form (Figure 8) again shows a constant concentration flux as a function of time from the concentration parallel to the time axis. The integrated plot (Figure 9), shown in cumulative mass form, demonstrates a near linear, zero-order plot representative of film evaporation. Therefore, two independent couplings of different wind tunnels and vapor analysis systems have demonstrated promising capabilities for environmental fate measurements. Note that the cumulative mass fraction consists of the analyzed vapor fraction and total mass balance methodology studies have not yet been finalized.

Figure 8. Evaporation of a Droplet of HD on Al in 5 cm Vapor Sampling Tunnel at 30 C and 0% RH for a 1.27mg, 1.24 mm Diameter Drop.

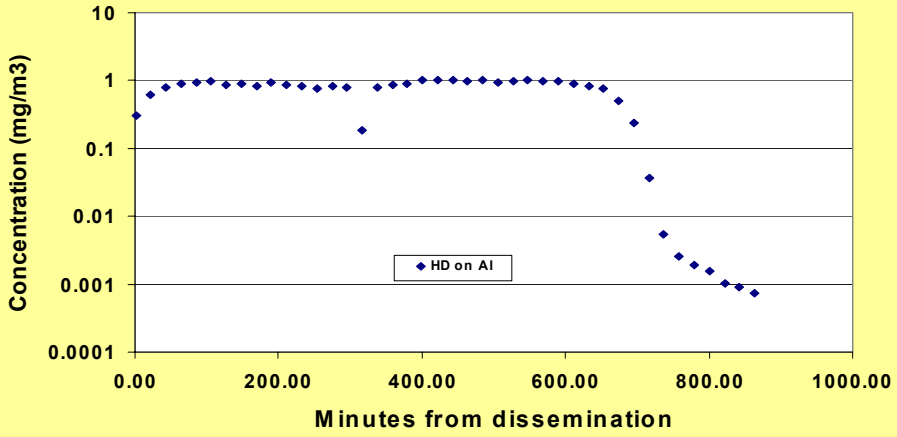
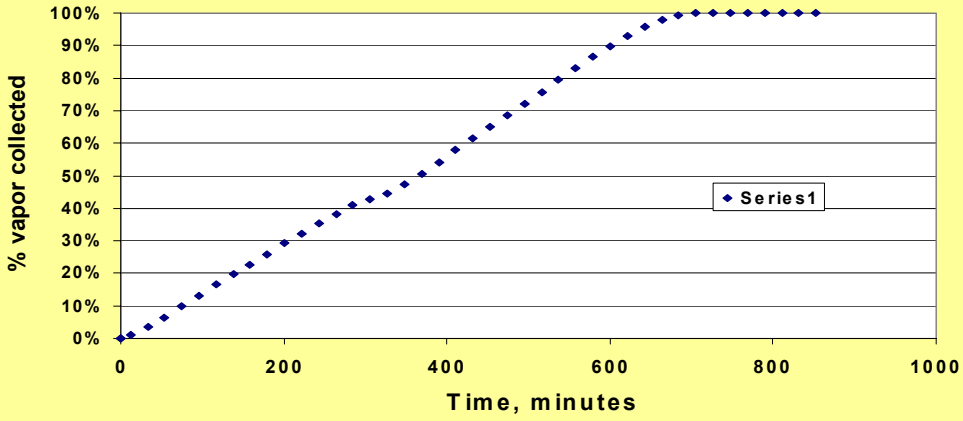


Figure 9. Mass of HD Evaporated and Collected, Calculated From the Concentration, Flow Rate, and Sample Period During an Experiment.



Wind Speed Methodology. In table 1 is collected the range of wind speeds for several wind tunnel cross-sections evaluated to date; the meters/second units are converted in miles per hour in parenstheses (mph). The first column lists the wind tunnel type, each characterized by a different cross-section and/or flow controller range. The second column list the range of nominal mean wind speeds, based on the flow rate range and cross-sectional area calculation. The third column lists the wind speed measured by hot wire anemometer at 0.254 mm from the surface containing the sorbed or sessile chemical agent droplet. Note that the wind speed over the entire wind tunnel height from surface to centerline was measured and only the closest distance to the surface at 0.254 mm is listed here. The first row lists the computed friction velocity range based on stability exponents of 0.1-0.3 in the Frost equation (1,4) and a range of 2-meter wind speeds from 0.5 to 10 m/s (based on 5 to 95 percentile frequencies, reported by co-investigators E. Ling and W. Fitzpatrick, STI). The next three rows contain the wind speeds for the 5-cm wind tunnel (5) with different flow controller systems that cover staggered ranges of wind speeds and/or vapor analysis strategies. Note that the high range of target wind speeds is covered by the voltage-calibrated blower system, the mid to low range is covered by the compressor driven environmental control system, and the lower range is bracketed by the total collection configuration, driven by pull from the thermal desorber pump. The microbalance wind tunnels cover the lower range of wind speeds (6). The measurement limits of the upper end of the wind speed range for the microbalance wind tunnels have not yet been finalized. Overall, no single system can cover the entire range of wind speeds and analytical concentrations; however, the range of wind speeds of interest can be covered by the spectrum of instrumentation and methodologies developed to date.

TABLE 1. Wind Speed Range for Environmental Fate Wind Tunnels, Meters/Second (MPH)

Wind Tunnel Mode	Mean Wind Speed Range	Drop Level Wind Speed Range (0.25 mm)
Friction Velocity Reference: Stability exponent 0.3 to 0.1	2 meter: 0.5-10 (1.1-22.3)	0.034-4.1 (0.076-9.1)
5-cm Total Collection	<0.0005-0.002 (0.001-0.0045)	<0.0005 non-stagnant
5-cm Compressor Controller (MN)	0.3-3.2 (0.7-7)	0.15-1.6 (0.33-3.6)
5-cm Calibrated Blower	1.8-7.4 (4-16.5)	1-4 (2.2-8.8)
Microbalance Model TA2950	0.13-1.75 (0.3-3.9)	<0.3-0.5 (0.7-1.1)
Microbalance Model TA 951	0.05-0.21 (0.12-0.47)	<0.05-0.1 (0.11-0.22)
Microbalance Model TA Q600	0.04-0.004 (0.01-0.1)	TBD

Analytical Methodology for a Spectrum of Surface Materials. Each combination of toxic contaminant and surface presents a challenge to the analytical methodology. A preliminary evaluation of the capability of the developed wind tunnels with respect to the various surfaces is summarized in table 2. One of the factors determining the applicability of an instrumental

approach to a surface was the geometry of the droplet on the surface. Therefore, the contact angle wind tunnel is not useful with droplets that immediately sorb into a substrate and a 'No' is found in these table elements; however, the contact angle instrument can provide the best measurement of the wetted area as a function of time for these sorbed droplets. Preliminary experiments indicate that chemical agent droplets will form sessile drops on the bitumen area of asphalt or tarmac, although the final geometry of this droplet-surface has not been determined for all agent combinations. The spread of chemical agents on the aggregate surface area of concrete and asphalt pavement was observed to occur as rapid, lateral film spreading before adsorption, therefore, the initial fate might be measured by contact angle wind tunnel. The measurement of agent droplet desorption into humid air from moisture adsorbing materials such as concrete and soil will depend on the resultant mass stability from the pre-conditioning of the specimen. The Model TA Q600 microbalance wind tunnel was developed because it had a reference beam that could cancel out moisture absorption. Overall, one or more wind tunnel analytical techniques is available for any of the environmental or other material types.

TABLE 2. Estimated Capabilities for Wind Tunnel Instrumentation for Monitoring Droplet Fate on Surfaces.

Surface	Microbalance TA951	Microbalance TA2950	Microbalance TAQ600	Vapor Analysis	Contact Angle
Glass	YES	YES	YES	YES	YES
Aluminum	YES	YES	YES	YES	YES
Coating	YES	YES	YES	YES	Initial
Concrete: aggregate	YES	YES	YES	YES	TBD
Concrete, cement	Low RH	Low RH	High RH TBD	YES	NO
Concrete, interface	Low RH	Low RH	High RH TBD	YES	NO
Tarmac: aggregate	YES	YES	YES	YES	TBD
Tarmac: asphalt	YES	YES	YES	YES	TBD
Tarmac: interface	YES	YES	YES	YES	NO
Soil	TBD	TBD	TBD	YES	NO
Leaf	YES	YES	YES	YES	YES
Plastic cargo cover	YES	YES	YES	YES	YES initial
Coated metal, aircraft	YES	YES	YES	YES	YES
Fiberglass, vehicle interior	YES	YES	YES	YES	YES
Rubber, tire	YES	YES	YES	YES	YES
Canvas	YES	YES	YES	YES	TBD
TBD: to be determined					

SUMMARY

Microbalance and vapor sampling wind tunnel analyses for chemical agents has been developed and appears feasible for most agent-material combinations and concentration ranges. Control and measurement of physical variables for moderate environmental temperature and humidity conditions is adequate. Droplet dosing accuracy appears adequate for 500 to 5000 micron diameter spherical droplets; droplet control below about 50 nanoliters requires further development. Overall, the toxic chemical wind tunnel methodologies developed to date appear to be capable of measuring agent fate over a significant spectrum of environmental conditions

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